

6-Mercaptopurine  
50-44-2 | DTXSID0020810

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 2.02e-11 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 2.21e-01

**Confidence level:** 6.12e-01

## Nearest Neighbors from the Training Set

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2,5-Furandione

**Measured:** 1.45e-12

**Predicted:** 2.17e-12

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2(3H)-Furanone

**Measured:** 4.45e-11

**Predicted:** 3.74e-11

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(2E)-2-Hexenal

**Measured:** 4.40e-11

**Predicted:** 4.31e-11